U.S. DEPARTMENT OF ENERGY | Nuclear Energy

NUCLEAR ENERGY ADVANCED MODELING & SIMULATION

The FUELS Integrated Performance & Safety Code

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Outline of Presentation

- **The Fuels IPSC**
  - Objectives for the Product
  - Multiscale, Multiphysics Approach
  - Synergy with the FCRD Advanced Fuels Campaign

- **Two Codes: AMP and MBM**

- **An Illustration: Challenge Problem(s)**

Objectives of the Fuels IPSC

- **The Fuels IPSC objective is to deliver a science-based (truly predictive) computational tool for nuclear fuel pin/assembly analysis and design**
  - Near term: oxide & metallic fuels, thermal & fast spectra (water & sodium coolants), irradiation performance of fuel pins in the quasi-steady state and operational transients
  - Longer term: additional fuel forms, irradiation performance of fuel pins/ assemblies during transients/accidents

- **Potential Applications**
  - LWRs: better informed safety margins, better informed operational constraints, power uprates, burnup extension
  - Advanced Reactors: (accelerated) design and qualification of new fuels

- **Customers/stakeholders**
  - CASL (LWRs)
  - FCRD (advanced reactors)

Multiscale, Multiphysics Approach

Approach: *Multi-scale, multi-physics based fuel performance simulations in 3D*

- Make use of theory/first principles, reduce reliance on empirical models
- Develop atomistically-informed meso-scale models to simulate evolution of microstructure under irradiation
- (Validate physics models vs. separate effects and integral experiments)
- Predict fuel properties and performance at engineering scale

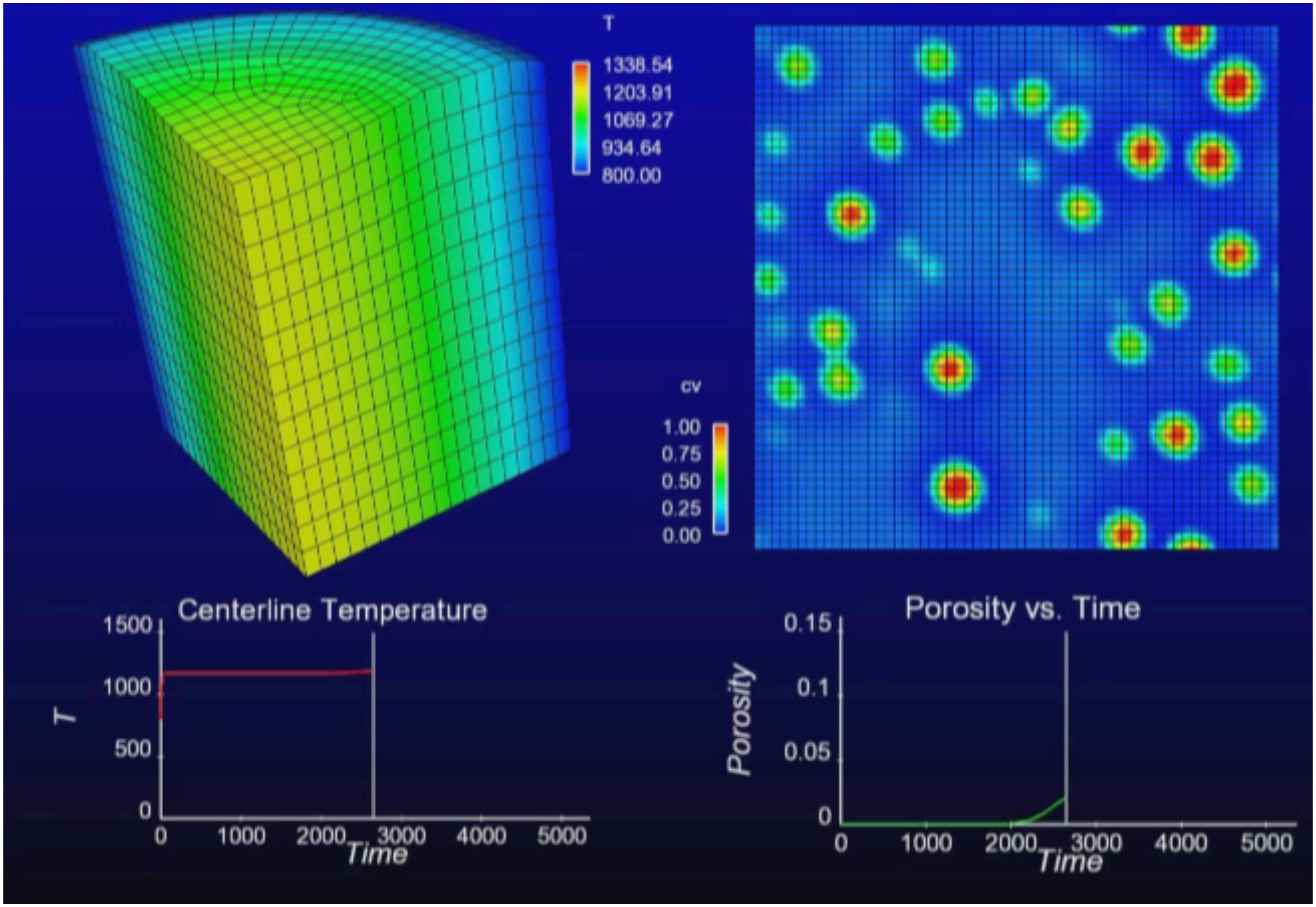
Lower Length Scale Physics

- Understand the thermodynamic and kinetic relationships between multi-dimensional materials/defect structures and predict their evolution under irradiation
- Up-scale results to inform engineering scale simulation

Irradiation Performance at Engineering Scale

- Simulate integral performance of fuels under irradiation
- Assess safety margins (including failure probabilities) with quantified uncertainties for normal operating conditions and transients
- Develop methodologies to optimize fuel designs/constrain reactor operations in order to minimize fuel degradation and avoid fuel failure

Evolving Microstructure used to Degrade Thermal Conductivity



Synergy with the FCRD Advanced Fuels Campaign

- **Advanced Fuels Campaign Execution Plan (FY10)**
  - **3** Areas of Emphasis in Irradiation Testing (FY11 - FY15)

1. Feasibility testing of emergent, innovative fuel concepts that address the "Grand Challenges".
2. Separate effects testing to broadly advance the theoretical understanding of nuclear fuel behavior and inform/validate the advanced modeling and simulation effort.
3. Assessments to gain an understanding of the differences and/or limitations between testing in neutron-shrouded positions in thermal test reactors vs. prototypic fast-spectrum environments.

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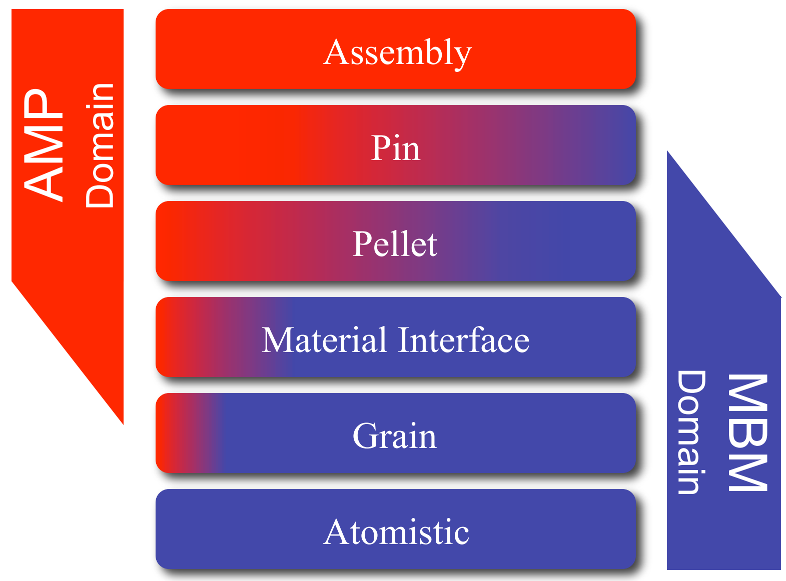
Two Codes: AMP & MBM

- **A Multiscale Problem**
  1) Assembly
  2) Pin
  3) Pellet
  4) Material Interface
  5) Grain
  6) Atomic

Meso-scale

Engineering Scale

Lower Length Scale



Target length scales for AMP vs. MBM applications; some overlap necessary.

- **AMP**
  - Focused on engineering scale simulations
  - Informed and validated by integral experiments
- **MBM (MOOSE-Bison-Marmot)**
  - Focused on meso-scale scale simulations and upscaling to pellet/pin
  - Informed and validated by separate effects experiments
- **Engineering & Meso-scale Coupled Simulations**
  - ☞ Potential for a truly predictive computational tool ! ! !

Fuels IPSC Challenge Problem(s)

- **For a full-size fuel pin, predict cladding integrity during steady-state reactor operation and anticipated, operational transients**

① **Oxide fuel in LWR (UO_2 in Zircaloy cladding)**

- ☑ Fuel swelling/fission gas release
- ☑ Cladding creep
- ☑ Pellet-cladding mechanical interaction
- ☑ Cladding corrosion/hydriding
- ➔ **Failure prediction** (with uncertainty estimate)

Champion: **Industry/CASL**

② **Metallic/oxide fuel in SFR (U-Pu-Zr/MOX in SS cladding)**

- ☑ Restructuring, constituent redistribution, solid fission product transport
- ☑ Fuel swelling/fission gas release
- ☑ Cladding creep
- ☑ Fuel-cladding mechanical interaction
- ☑ Fuel-cladding chemical interaction
- ➔ **Failure prediction** (with uncertainty estimate)

Champion: **FCRD**

Challenge Problem(s) Context

- **What's <u>not</u> new, different?**
  - Fuel systems (UO_2, MOX, U-Pu-Zr fuels; Zircaloy, SS claddings)
  - Reactor systems (LWR, SFR)
- **What's new, different, better?**
  - Reactor operations (power, temperature, burnup, ramp rate)?
    - *e.g., failure probability vs. ramp rate, cladding/coolant temperature, burnup*
    - *This could be of real value to reactor operators, leading to power uprates, relaxation of operation constraints that come from fuel concerns (e.g., PCI), burnup extension...*
  - Science-based performance models that enable true predictability outside empirically derived (operational) database
    - *Atomistically-informed simulations of microstructural evolution (lower length scale)*
    - *Properties and performance upscaled to engineering scale*